Endo-fullerenes and Doped Diamond Nanocrystallite based Solid-State Qubits

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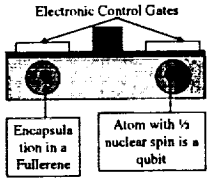
Background: Kane's Model of Solid-State Quantum Computers

- Solid state quantum computer: Arrays of phosphorus atoms in bulk Si, controlled by electronic gates using hyperfine interactions [1]
- Problem: Uniform arrays of individual dopant atoms in bulk Si are experimentally difficult !

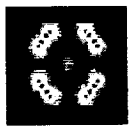
1. Kane, B.E., *Nature*, 393, p.133 (1998)

Solution: Use Encapsulated Atoms as Qubits !



Proposal: Arrays of "encapsulated" atoms (with ½ nuclear spin – qubits) will be easy to fabricate as compared to the arrays of the similar bare atoms.

Example: ^{1}H encapsulated in C_{36}



Electronic charge density shows a weak meta-stable state of ^{1}H at the center of C_{36}

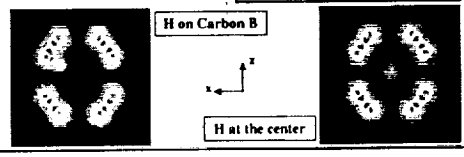
Suitable Solid-state Qubits Identified:

- ^{1}H encapsulated in a $C_{20}D_{20}$ fullerene
- ^{31}P encapsulated in a diamond nanocrystallite

Example: ^{1}H Encapsulated in C_{36}

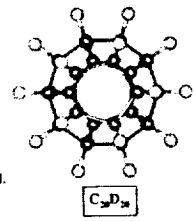
- Center is meta-stable site.
- ^{1}H strongly prefers to make a bond with a carbon atom

	Formation Energy (eV)
Carbon A	-1.28
Carbon B	-1.54
Carbon C	-1.40
Center	-0.46



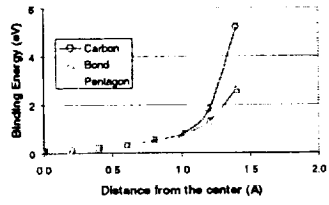
Reactivity Control for ^{1}H: $C_{20}D_{20}$

- ^{1}H prefers to make a bond with C atom within fullerene.
  → Reduce the chemical reactivity
- sp^3 hybrid will reduce the electron density of inner surface.
  → Hydrogenation
- Hexagon has lower diffusion barrier than pentagon.
  → Non-hexagon structure is preferred.
- As a conclusion, we examined $C_{20}D_{20}$



^{1}H Encapsulated in $C_{20}D_{20}$

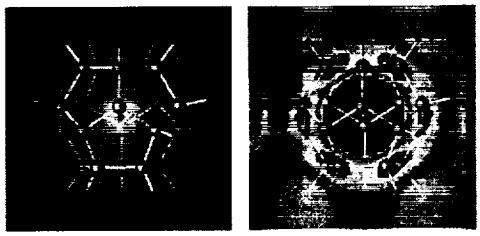
- Energy changes as moving ^{1}H from the center to the wall of $C_{20}D_{20}$



- Symmetry sites: Carbon, Bond, and Pentagon
- Center is the most stable site.
- No meta-stable site
- Diffusion Barrier ~ 1.17 eV

Charge Density of ^1H Encapsulated in $C_{20}D_{20}$

- Some of electron wave of ^1H is found out of $C_{20}D_{20}$

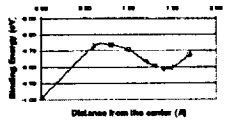


Model 2: Doped Diamond Nanocrystallite
Step1: ^{31}P Encapsulation in C_{60}

- Center is the most stable site for ^{31}P
- Diffusion barrier to move to a wall C atom is about 0.35 eV

^{31}P in C_{60}

	Formation Energy (eV)
(6,6) Bond	-0.81
Center	-0.99

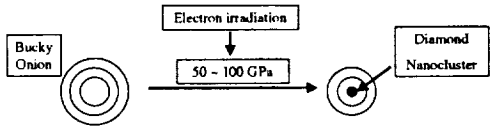


- Implantation of ^{31}P in a C_{60} fullerenes has been experimentally done !

Knapp, C et al. *Molecular Physics* 95, 999-1004 (1998).

Steps 2-3: Convert to a ^{31}P Encapsulation in a Diamond Nanocrystallite

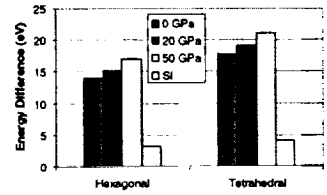
- Step2: grow bucky-onion layers with ^{31}P@ C_{60} fullerenes as seed material
- Step3: e-beam irradiation of the bucky-onion layers converts the core shells into ^{31}P doped in a diamond nanocrystallite



Banhart, F. and Ajayan, P.M., *Nature*, 382, p. 443 (1996)

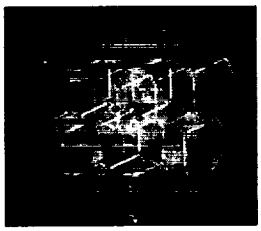
^{31}P doping in Diamond or Silicon

- Energy difference between ^{31}P at substitutional site, and two types of interstitial site of compressed diamond (0, 20, and 50 GPa) and bulk Si

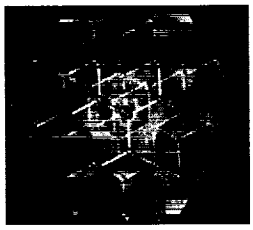


- Substitutional site is more stable than interstitial site.
- Diamond has bigger energy differences than Si.

Charge Density of ^{31}P in Diamond or Silicon



^{31}P in Diamond



^{31}P in Si

^{31}P in a Diamond Nanocrystallite as a Qubit (Comments)

- ^{31}P at a substitutional site in a diamond nanocrystallite is more stable (by -15 eV) than a ^{31}P at an interistitial site ~ no diffusion
- Spin-orbit interaction on a qubit is 8 times stronger than Kane's model
- In principle any host lattice can be chosen to tune the neighboring qubit interactions
- Experimentally feasible fabrication pathway for these solid-state qubits (Steps 1-3) exist